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Abstract. Distorted-wave Born approximation (DWBA) calculations are reported for singly-differential and total cross sections for the electron impact ionisation for atomic hydrogen at 25, 40, 60, 100, 150 and 250 eV. The theory is compared with available experiments. At all the energies except 25 eV the theory predicts a lower singly-differential cross section for the low-energy side of the secondary-electron energies (<5 eV), compared to the only available absolute measurements of Shyn (1992). The DWBA calculation is in good agreement with the experiment at 25eV but only if e-e post-collision interaction is included in the theory in some way.

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The problem of electron scattering on atomic hydrogen is often used in the investigation of various theoretical methods for electron-atom scattering. This

problem is very interesting from any point of view, for example as the simplest three body problem. It thus provides a substantial challenge for theory.

Due to its vital importance to the theory as well as to various practical applications, the total ionisation cross section has been measured as a function of energy with great accuracy by Shah *et al* (1987). These results are very important as they provide quite a reliable test of any electron-atom scattering theory. For example, they have been used by Bray *et al* (1991a) to test various approximations for the *ab initio* optical potential for later use in electron-atom scattering problems (Bray *et al* 1991b).

The experimental data of Shah *et al* (1987) are not absolute. They are normalised to the first Born approximation at high energy, see Shah *et al* (1987) for details. On the other hand the absolute measurements of Shyn (1992) have been reported recently and they predict larger total ionisation cross sections at 60 eV and higher, up to 250 eV. This discrepancy between the two experiments must be clarified.

In this letter we report distorted-wave Born approximation (DWBA) calculations for the singly-differential and total ionisation cross sections in the range of low to intermediate energies. The calculations have been mainly motivated by the new experimental results of Shyn (1992), the discrepancy between the two experiments noted above and the fact that the best available theoretical calculations for these cross sections are based on the plane-wave Born approximation which is only valid at very high incident energies (Shah *et al* 1987, McCarrol 1957).

The present DWBA calculations are improved over the previously-used distorted-wave calculations (Madison *et al* 1989, McCarthy and Zhang 1990 and Zhang *et al* 1990) by including the proper exchange part of the static-exchange potential of the atom which is important at low energies (Konovalov and McCarthy 1992, Bray *et al* 1991a). These improved DWBA calculations have been successfully used to describe the absolute measurements (Gélébart and Tweed 1990) of the electron impact ionisation of helium in coplanar-symmetric kinematics at 100eV (Konovalov and McCarthy 1992).

The fully-differential cross section for the $\text{H}(\epsilon, 2e)$ process is given by

$$\frac{d^5\sigma}{d\Omega_a d\Omega_b dE_a} = (2\pi)^4 \frac{k_a k_b}{k_0} \left(\frac{3}{4} |f_1|^2 + \frac{1}{4} |f_0|^2 \right). \quad (1)$$

The singly-differential cross section is

$$\frac{d\sigma}{dE_a} = \int \int d\Omega_a d\Omega_b \frac{d^5\sigma}{d\Omega_a d\Omega_b dE_a}, \quad (2)$$

where, in *post* form, the singlet ($S=0$) and triplet ($S=1$) amplitudes are given by

$$f_S = \langle \psi^{(-)}(\mathbf{k}_a, \mathbf{k}_b) | V | \Psi_{0,S}^{(+)}(\mathbf{k}_0, 1, 2) + (-1)^S \Psi_{0,S}^{(+)}(\mathbf{k}_0, 2, 1) \rangle, \quad (3)$$

where $\Psi_{0,S}^{(+)}(\mathbf{k}_0)$ and $\psi^{(-)}(\mathbf{k}_a, \mathbf{k}_b)$ are the solution of the Schrödinger equations

$$(H - E^{(+)}) \Psi_{0,S}^{(+)}(\mathbf{k}_0, \mathbf{r}_1, \mathbf{r}_2) = 0, \quad (4)$$

$$(H - V - E^{(-)}) \psi^{(-)}(\mathbf{k}_a, \mathbf{k}_b, \mathbf{r}_1, \mathbf{r}_2) = 0. \quad (5)$$

Here H is the total Hamiltonian of the system, V is the electron-electron potential.

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (6)$$

To calculate $\Psi_{0,S}^{(+)}(\mathbf{k}_0)$ we use the distorted-wave Born approximation

$$\Psi_{0,S}^{(+)}(\mathbf{k}_0, \mathbf{r}_1, \mathbf{r}_2) \approx \xi_S^{(+)}(\mathbf{k}_0, \mathbf{r}_1) \phi_{1s}(\mathbf{r}_2), \quad (7)$$

where ϕ_{1s} is the $1s$ orbital of $H(1s)$ and $\xi_S^{(+)}(\mathbf{k})$ is the distorted wave for the incident electron generated in the static-exchange potential of the atom.

For the wave function $\psi^{(-)}(\mathbf{k}_a, \mathbf{k}_b)$ we consider two different approximations. The first one has the space-dependent part

$$\psi^{(-)}(\mathbf{k}_a, \mathbf{k}_b, \mathbf{r}_1, \mathbf{r}_2) \approx \chi^{(-)}(\mathbf{k}_a, \mathbf{r}_1) \chi^{(-)}(\mathbf{k}_b, \mathbf{r}_2), \quad (8)$$

and the second one is

$$\psi^{(-)}(\mathbf{k}_a, \mathbf{k}_b, \mathbf{r}_1, \mathbf{r}_2) \approx \chi^{(-)}(\mathbf{k}_<, \mathbf{r}_1) \varphi(\mathbf{k}_>, \mathbf{r}_2), \quad (9)$$

where $\chi^{(-)}(\mathbf{k})$ is a Coulomb wave and $\varphi(\mathbf{k})$ is a plane wave orthogonalised to the ground state of the atom ϕ_{1s} . Subscripts $<, >$ indicate the slow and fast electron. This approximation has been developed for various coupled-channels optical calculations (Bray *et al* 1991a, 1991b) in order to include the interaction between the two electrons in the continuum. The interpretation of this approximation is as follows. The slower-moving electron feels the whole charge of the ion while the faster-moving electron feels zero charge at large distances, since the ion is screened by the slow electron. Orthogonalisation to the ground state is a computationally-tractable way of making this distorted wave more realistic in the optical potential calculation.

In figure 1 we compare our results for the singly-differential ionisation cross section with the absolute measurements of Shyn (1992). In figure 2 we

present DWBA results for the total ionisation cross section in comparison with the two experiments of Shyn (1992) and Shah *et al* (1987).

The measurements of Shyn give higher ionisation cross sections at 60, 100, 150 and 250 eV in comparison with the data of Shah *et al* (1987) (Figure 2). Since the standard deviation of the latter experiment (not shown on Figure 2 as it is smaller than the drawn symbol) is much less than that of Shyn, we would like to suggest that the former experiment overestimates this cross section. In Figure 1 the DWBA calculation predicts a lower singly-differential cross section for the low energy region of secondary electrons. At the same time both DWBA calculations become asymptotically the same in the region where the first Born approximation works well ($E_a > 250\text{eV}$) and the results are in good agreement with the experiment of Shah *et al* (1987). The discrepancy between these two most recent experiments will require further investigation.

At 25 eV the two experiments are in complete agreement with each other (Figure 2). This makes the experimental data on Figure 1 (25 eV) especially interesting. These data are well described (almost within one standard deviation) by the second approximation of $\psi^{(-)}(\mathbf{k}_a, \mathbf{k}_b)$ (9) while the first approximation (8) is clearly inadequate at this low energy. The first approximation comes from the standard scattering theory for the chosen scattering potential (6). It does not include any post-collision e - e interaction in any form. On the other hand, the second approximation of $\psi^{(-)}(\mathbf{k}_a, \mathbf{k}_b)$ includes post-collision interaction between two electrons, although not explicitly. Our results at 25

eV confirm the suggestion (Jones *et al* 1992, Pan and Starace 1992, Rösel *et al* 1992) that a DWBA calculation could reproduce results of $(e,2e)$ experiments even at quite low incident energies but with one important condition: the post-collision interaction must be incorporated into a DWBA calculation in some way.

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Figure captions

Figure 1. Singly-differential cross sections ($d\sigma/dE_a$) of the electron impact ionisation for atomic hydrogen. The solid line is the DWBA calculation which includes post-collision interaction, see (9) in the text. The short-dashed line omits any post-collision effects, see (8) in the text. The absolute measurements of Shyn (1992) are denoted by \odot .

Figure 2. Total ionisation cross sections of atomic hydrogen by electron impact. For details of notation see figure 1. The experimental points Δ are due to Shah *et al* (1987).

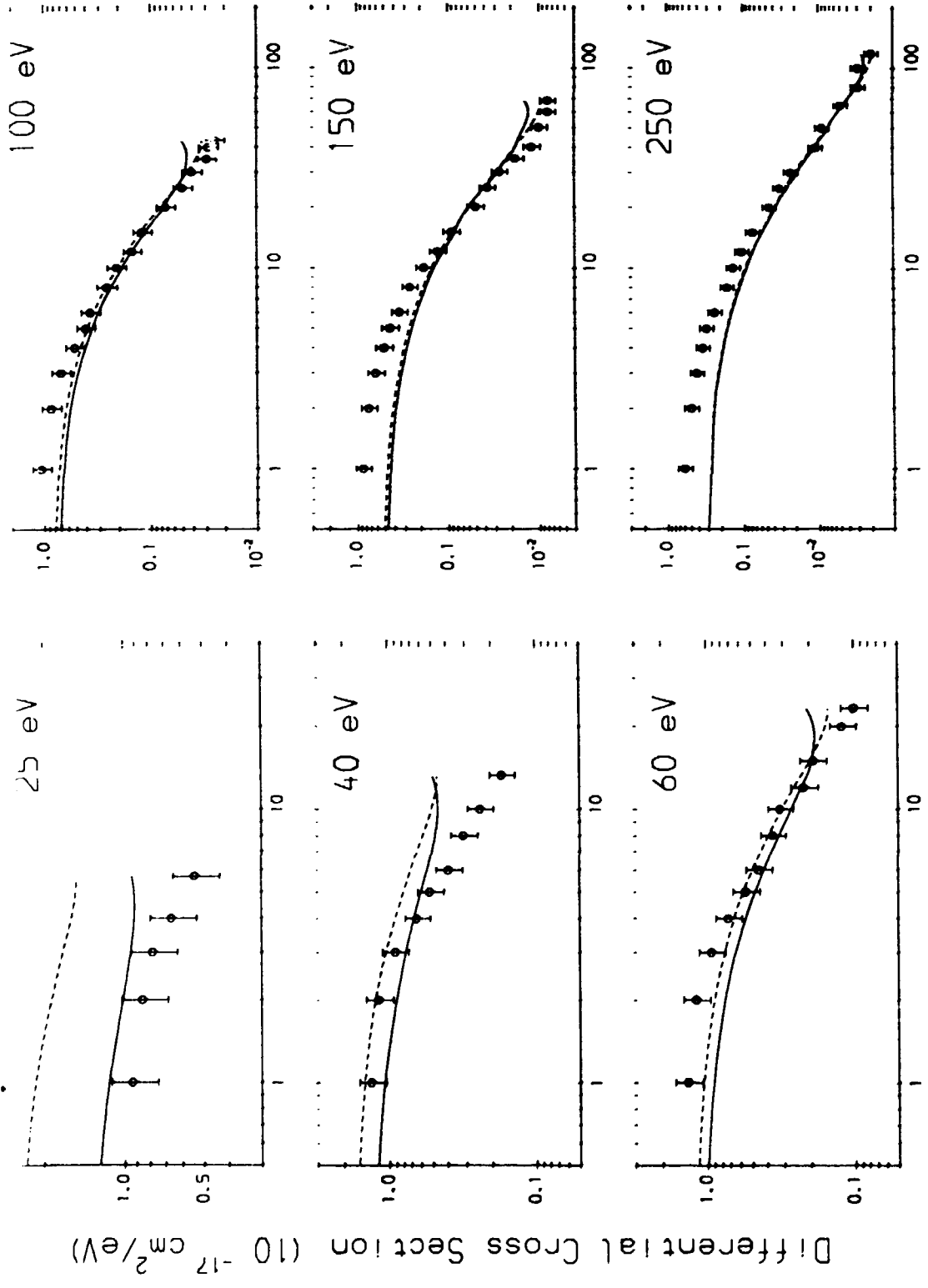


Fig. 1

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Secondary-electron energy (eV)

Differential Cross Section ($10^{-17} \text{ cm}^2/\text{eV}$)

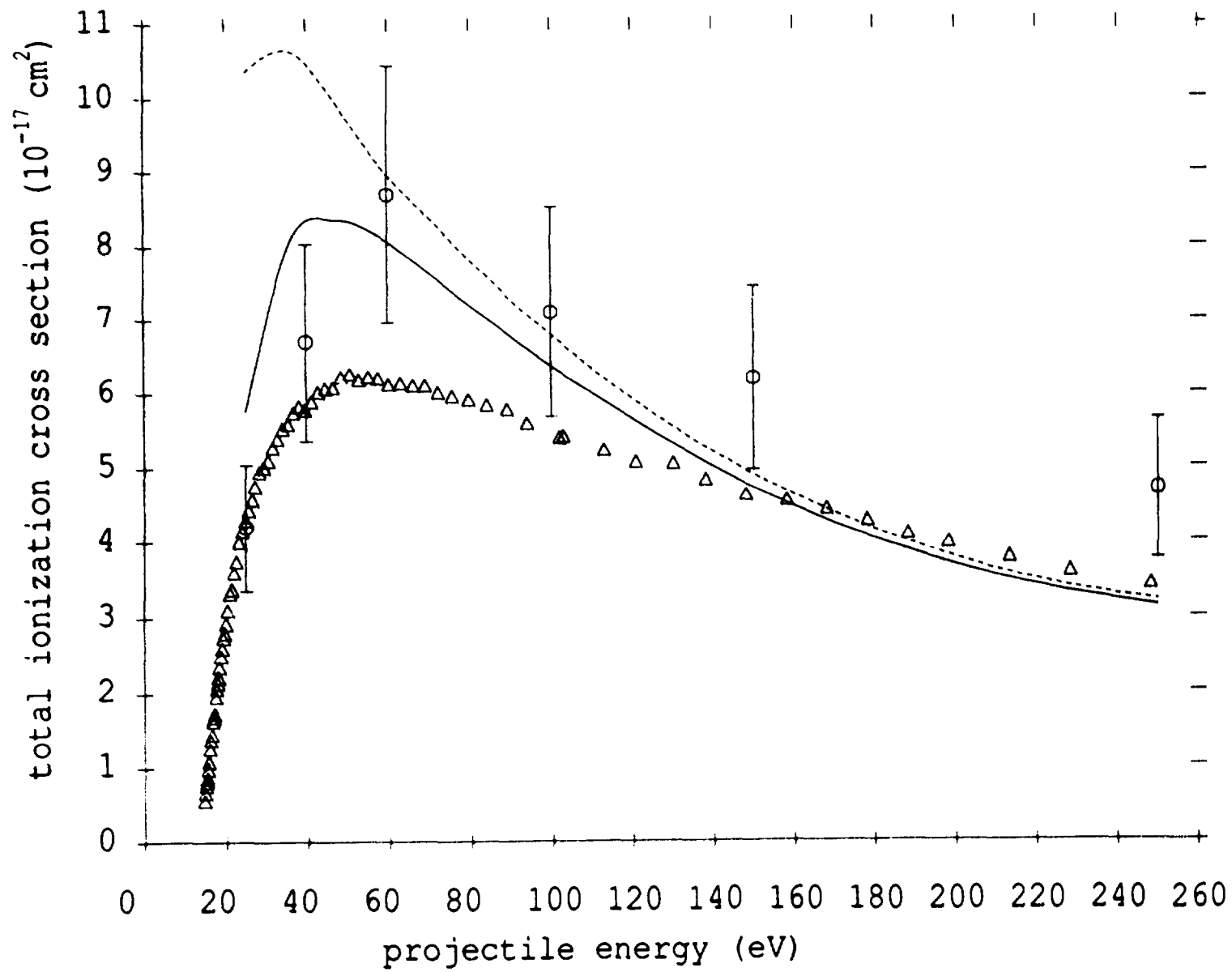


Fig.2

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